

Supplemental Material for "¹H-¹³C Dipole-Dipole Cross-Correlated Spin Relaxation as a Probe of Dynamics in Unfolded Proteins: Application to the drkN SH3 Domain"

Supplemental Table 1:

Amino Acid	F_{exch}		U_{exch}		U_{Gdn}	
	$\Gamma_{\text{HC1,HC2}}^a$	Error	$\Gamma_{\text{HC1,HC2}}$	Error	$\Gamma_{\text{HC1,HC2}}$	Error
E2	-11.8	0.6	-3.6	0.1	-3.3	0.1
K6	-7.2	0.7	b		-2.8	0.1
H7	-14.0	0.4	-7.0	0.1	-4.9	0.1
D8	-24.8	0.7	-7.4	0.1	-5.6	0.1
F9	-25.4	0.8	-5.6	0.1	-5.1	0.1
S10	-1.4	0.4	-2.9	0.1	-3.3	0.1
D14	-9.6	0.2	-7.2	0.1	-4.8	0.1
D15	-14.5	0.3	-9.3	0.2	-6.1	0.1
E16	-20.2	2.0	-7.1	0.6	-5.4	0.1
L17	-9.8	1.3	-5.9	0.8	-5.9	0.1
S18	-18.5	0.9	-3.0	0.9	-2.6	0.1
F19	-27.6	1.4	-15.3	1.7	-6.9	0.1
R20	-15.6	1.0	-4.8	0.6	-6.9	0.2
K21	-4.8	1.1	-1.6	1.4	-4.2	0.2
Q23	-16.0	1.5			-6.2	0.2
L25	-21.8	1.1			-8.1	0.2
K26	-2.3	0.8			-4.1	0.2
L28	-20.2	1.3			-7.0	0.2
N29	-15.0	0.7	-2.0	1.2	-5.6	0.1
M30	-6.0	0.7	-8.7	1.1	-7.6	0.2
E31	-12.6	0.5			-6.8	0.1
D32	-10.7	0.3	-8.3	0.4	-7.1	0.1
D33	-14.6	2.9	-9.8	0.3	-6.9	0.1
S34	-5.2	0.6	-2.9	0.2		
N35	-13.3	0.6	-7.4	0.4	-5.2	0.1
W36	-17.5	1.3	-21.9	2.3	-10.8	0.2
Y37	-21.8	1.5	-15.2	1.2	-11.3	0.1
R38	-8.5	1.1	-6.8	0.9	-7.9	0.2
E40	-14.6	0.8	-8.9	0.6	-8.2	0.1
L41	-21.6	2.8	-7.1	0.6	-7.6	0.2
D42	-4.7	0.3	-6.9	0.2	-5.6	0.1
G43	-23.6	0.3	-5.2	0.1	-1.9	0.1
K44					-4.0	0.1
E45			-5.7	0.2		
G46	-33.4	0.9	-5.3	0.1	-2.6	0.1
L47	-15.6	2.3	-4.1	0.5	-6.1	0.2
P49	-6.6	2.6	-4.8	0.5	-3.7	0.2
S50	-17.0	0.7				
N51	-11.3	0.4	-6.5	0.2	-5.0	0.1
Y52	-22.2	1.3	-10.4	0.2	-8.3	0.1
E54	-1.6	0.5	-4.1	0.2	-5.4	0.1
K56			-2.5	0.1	-2.8	0.1

N57	-3.7	0.1	-3.4	0.1
H58			-3.2	0.1

^aValues in s⁻¹

^bNo data available

Supplemental Table 2. $^3J_{C'C\gamma}$, $^3J_{NC\gamma}$ coupling values of aromatic residues in the U_{exch} and F_{exch} states of the drkN SH3 domain measured according to the method of Hu et al²².

	F_{exch}		U_{exch}	
	$^3J_{C'C\gamma}$ (Hz) ^a	$^3J_{NC\gamma}$ (Hz) ^a	$^3J_{C'C\gamma}$ (Hz) ^a	$^3J_{NC\gamma}$ (Hz) ^a
H7	3.0	1.1	3.0	1.2
F9	< 1.4	b	2.6	0.9
F19	c	0.5	b	b
W36	4.3	$ ^3J_{NC\gamma} < 0.4$	2.3	1.1
Y37	3.3	0.3	2.0	1.3
Y52	2.7	$ ^3J_{NC\gamma} < 0.3$	1.8	$ ^3J_{NC\gamma} < 1.4^d$
H58	2.3	1.0	2.0	0.9

^aErrors of ≈ 0.1 Hz are calculated based on the rmsd noise.

^bIntensity could not be measured due to spectral overlap.

^cCorrelation not observed in spectrum.

^dPartial overlap of amide resonance with E31.

Supplemental Figure 3. $\Gamma_{\text{HC1,HC2}}$ values for the F_{exch} (a), U_{exch} (b) and U_{Gdn} (c) states.

